ABSTRACT

DISSERTATION/THESIS/RESEARCH PAPER/CREATIVE PROJECT: Measuring the Quality of Generalized Gradient Approximations in a Density Functional Theory Pseudopotential Enviroment for Solids

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The ability to model ground-state properties in density function theory (DFT) is affected by the theoretical treatment of the electrons and the numerical approach to the theory. The electron-electron interaction energy is approximated by exchange-correlation (XC) functionals which are functions of the electron density. Popular functionals include the localized density approximation (LDA) or one of many generalized gradient approximations (GGA). The numerical approaches used are the core-electron approximating pseudopotential (PsP) or the more accurate all-electron (AE) method. We test whether PsP calculations for some new GGA's can accurately reproduce AE values for cohesive energy, lattice constant, and bulk modulus for sixteen solids. We compare our PsP results to AE results for several XC functionals and gauge the quality of functionals by comparison to experiment. This allows us to determine which errors are caused by functionals and which are caused by PsP's.